Bisphenol B
77-40-7 | DTXSID4022442

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 337 °C

Global applicability domain: Inside

Local applicability domain index: 3.06e-01

Confidence level: 5.77e-01

Nearest Neighbors from the Training Set

Image not found
2,2'-Dihydroxybenzophenone
Measured: 333
Predicted: 318

Image not found
(1,1'-Biphenyl)-2,2'-diol
Measured: 320
Predicted: 315

Image not found
4-Hexylresorcinol
Measured: 334
Predicted: 302

Image not found
Alizarin
Measured: 430
Predicted: 399

Image not found
tert-Butylhydroquinone
Measured: 273
Predicted: 277